Simazine

122-34-9 | DTXSID4021268

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.97

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 6.10e-01

Nearest Neighbors from the Training Set

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Simazine
Measured: 2.18
Predicted: 1.97

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Atrazine
Measured: 2.61
Predicted: 2.67

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Ethanol, 2-[[4-chloro-6-[(1-methylethyl)amino]-1,3,5-triazin-2-yl]amino]-
Measured: 0.78
Predicted: 1.80